1D 1H NMR with on non-deuterated solvents ("no-D")

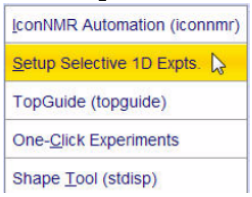
Without deuterium, the magnet field cannot be locked and on our older magnets, the field moves with each scan. Because of this, 1H NMR without deuterium lock only works well on two NMR instruments: the 400SL and the 500 Ascend.

1. The lock and sweep must be off. After your sample is inserted, do not type **lock**, but instead type **lopo**. In the BSMS window, select the [Lock/Level] tab and turn off both lock and sweep. The sweep and lock buttons should NOT be green. If they are green, click the relevant On-Off button.
2. Take a normal 1D spectrum, but with ns=1 and rg=1. (Type **rpar protonstd all** and then **ns=1** and **rg=1** and then **zg** or **start**). Process and note the shift(s) of your solvent peak(s).
3. To shim, you can use the 1H selective Topshim function. Type **topshim lockoff 1h o1p=#** in the command line where # is the ppm of largest solvent peak. If there is more than one peak, append **selwid=0.5** to the command above.
4. If desired, you may retake your spectrum to see the improvement in resolution. If your sample is concentrated enough, this spectrum may be sufficient.

To suppress the protonated solvent signal, follow the Selective 1D Proton handout:

5. Go to the **[Acquire]** menu and select **[More]**.

6. Choose **[Setup Selective 1D Experiment]** under the drop down menu.

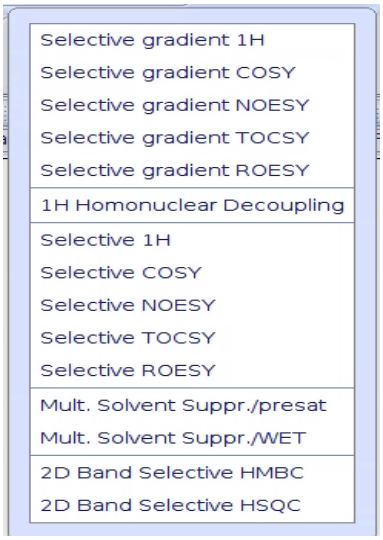


7. A new menu will appear and flash briefly:

8. select 

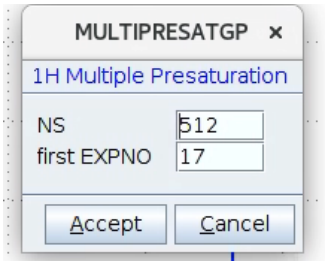
and Topspin goes into integration mode.
9. Integrate the solvent peak(s), but define the integral region very narrowly, such that no extra baseline is included (this is different from an actual integral) then select  and **[Save Regions to 'reg']**, then exit  . Answer **[no]** to the question about saving regions.
10. Select 

and choose Mult. Solvent Suppr. WET from the list, as shown below. You may also choose Mult. Solvent Suppr. Presat but WET works better.

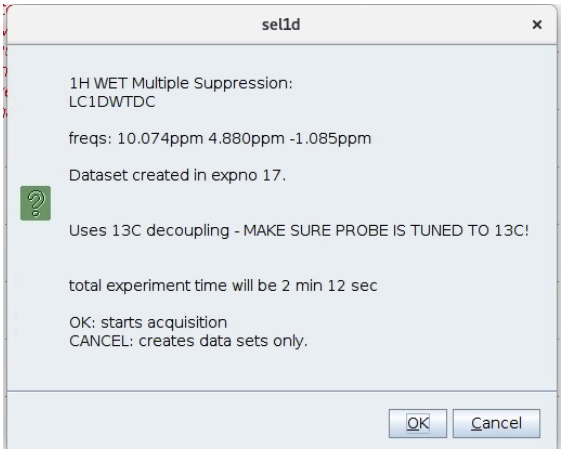


For WET solvent suppression, a special shaped excitation pulse is created that attempts to suppress all solvents peaks (2 is the practical maximum) at the same time in a single experiment.

11. You will get a window asking for the parameter NS and EXPNO. Adjust NS. Usually 32 is sufficient. Click Accept.



A message titled “sel1d” is displayed. Sometimes the 13C satellites of the solvent are a nuisance in the 1H suppressed spectrum. WET suppression includes 13C decoupling to collapse and suppress them. For this to work, the 13C channel of the probe must be tuned.



12. If this is not important to you, click OK and the spectrum will be acquired.
13. If suppressing the satellites are important to you, click Cancel and navigate to the expno indicated in the message. Then type **atma f2.** When atma is finished, navigate back to the original expno and type start.